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LDRD Final Report: Surrogate Nuclear Reactions and the Origin of the Heavy Elements (04-ERD-057)

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FY06 LDRD Final Report

Surrogate Nuclear Reactions and the Origin of the Heavy Elements

04-ERD-057

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Abstract

Research carried out in the framework of the LDRD project "Surrogate Nuclear Reactions and the Origin of the Heavy Elements" (04-ERD-057) is summarized. The project was designed to address the challenge of determining cross sections for nuclear reactions involving unstable targets, with a particular emphasis on reactions that play a key role in the production of the elements between Iron and Uranium. This report reviews the motivation for the research, introduces the approach employed to address the problem, and summarizes the resulting scientific insights, technical findings, and related accomplishments.

Contents

1 Introduction

Determining reaction cross sections on unstable nuclear species is a major challenge for nuclear physics and nuclear astrophysics. Many of these nuclei are too difficult to produce with currently available experimental techniques or too short-lived to serve as targets in present-day set-ups. Some nuclear reactions will remain unmeasurable even at upcoming and planned radioactive beam facilities. It is therefore important to explore alternative methods for determining reaction cross sections on unstable nuclei. The research carried out in the framework of this LDRD project has focused on the "Surrogate Nuclear Reaction Technique", an indirect method for determining compound-nuclear reaction cross sections. Surrogate experiments employ reactions different from but related to the desired reaction and can thus often avoid the difficulties associated with extremely short-lived target nuclei.

The goal of this LDRD project was to develop the theoretical and experimental framework for planning and analyzing Surrogate experiments that provide cross section information for reactions involving unstable targets, with a particular focus on reactions involving unstable nuclei that play a key role in the production of the elements between Iron and Uranium. Below we outline the astrophysical context and motivation for our work, briefly review the Surrogate concept and associated challenges. A summary of our research goals and activities during this LDRD project is given in Section 2. Representative findings that resulted from our work are discussed in Section 3. Additional accomplishments (presentations and publications, training and recruiting, building collaborative efforts, workshop organization, etc.) are given in Section 4. Some remarks regarding follow-on funding can be found in Section 5.

1.1 Astrophysical context and motivation for the work

Nuclear astrophysics addresses some of the most compelling questions in nature: What are the origins of the elements necessary for life? What is the age of the universe? How did the sun, the stars, our galaxy, form and evolve? Over the past 75 years we have acquired a basic, but incomplete, understanding of the processes that generate the energy in stars such as our sun, that drive the evolution of stars and that are responsible for the synthesis of the elements. New astrophysical observations and recent progress in experimental techniques, coupled with an emerging generation of sophisticated models of astrophysical phenomena, present a unique opportunity for significant advances in our knowledge of the cosmos. Among the unanswered mysteries about the nature and evolution of our universe is the origin of the heavy elements. The question "How were the elements from Iron to Uranium made?" appears in every survey of nuclear astrophysics challenges and has been identified as one of the "Eleven Science Questions for the New Century" in the recent "Connecting Quarks to the Cosmos" report by the National Research Council's Board on Physics and Astronomy [31]. The desire to answer this question is a major motivation for the study of unstable nuclei. Such studies are pursued at a variety of existing radioactive beam facilities around the world. Building a major new facility dedicated to the exploration of unstable nuclei, their properties and reactions with each other has been a top priority for the DOE and the nuclear science community [24, 14, 1, 16, 35].

It is well known that nucleosynthesis of heavy elements beyond ^{56}Fe takes place almost exclusively by neutron capture on lighter seed nuclei in the s and r processes [11, 39, 36]. The ("slow") s process takes place under conditions in which the time interval between successive neutron captures is longer than the average life time for β-decay. As a result, the s process proceeds through nuclides in and very near the valley of stability. The ("rapid") r process, in contrast, takes place in an environment with high temperature (T $> 10^9$K) and high neutron density ($\rho > 10^{20}/\mathrm{cm}^2$), such as a supernova. In such conditions the average time between neutron captures is much shorter than the life time for β-decay and reaction flows can proceed to very neutron-rich nuclei. When the strong neutron flux subsides, these neutron-rich nuclei decay back towards the valley of stability and produce relative isotopic abundances characteristic of the process ("r-process abundances"). Since very little is known about the r process, its abundances are inferred by subtracting calculated s-process abundances from measured total abundances. Until recently, rather schematic s-process models reproduced the known s-process abundance patterns fairly well. However, with more precise astronomical observations and improved stellar models available, progress in understanding the s process (and thus in understanding the inner workings of stars and galactic chemical evolution) is now limited due to the lack of good neutron-capture data [24, 14, 29]. Of particular interest are s-process branch points, unstable nuclei that are produced in the s process with a life time long enough to allow the s process to proceed by either neutron capture or β decay. A very important ingredient for determining the probability of one path dominating over the other is the associated neutron-capture cross section. One objective of the LDRD project has been to investigate the possibilities of obtaining neutron-capture cross sections for s-process branch-point nuclei via the Surrogate method.

Exploring the physics of unstable nuclei has been identified as a major objective in the Laboratory's Science and Technology Plan [2]. Such exploration is not only relevant to basic nuclear physics and astrophysics. Important applications in the areas of Stockpile Stewardship, Homeland Security, and nuclear energy require reliable information on reactions involving unstable nuclei. Since many reactions of interest will remain to elusive, even at existing and planned radioactive beam facilities, it is crucial to develop indirect approaches such as the Surrogate method. Prior to the LDRD project, the Surrogate method was primarily used to estimate (n,f) cross sections for various actinide targets. Moreover, applications of the method typically used approximations that were not well studied. It thus became important to examine the limitations of the Surrogate approach in general and of the approximations commonly employed in particular. The primary approximation, the use of the Weisskopf-Ewing limit, is explained in the next section. Some of our findings regarding the validity of the Weisskopf-Ewing approximation are discussed in Section 3.2.

1.2 The Surrogate approach

The Surrogate Nuclear Reaction technique combines experiment with theory to obtain cross sections for compound-nuclear reactions, $a+A \rightarrow B^* \rightarrow c+C$, involving difficult-to-produce targets, A. In the Hauser-Feshbach formalism [28], the cross section for this "desired" reaction takes the form:

$$\sigma_{\alpha\chi}(E_a) = \sum_{J,\pi} \sigma_\alpha^{CN}(E_{ex}, J, \pi) \; G_\chi^{CN}(E_{ex}, J, \pi) \; , \tag{1}$$

with α and χ denoting the relevant entrance and exit channels, $a + A$ and $c + C$, respectively [28]. The excitation energy E of the compound nucleus, B^*, is related to the projectile energy E_a via the energy needed for separating a from B: $E_a = E - S_a(B)$. In many cases the formation cross section $\sigma_\alpha^{CN} = \sigma(a+A \to B^*)$ can be calculated to a reasonable accuracy by using optical potentials, while the theoretical decay probabilities G_χ^{CN} for the different decay channels χ are often quite uncertain. The latter are difficult to calculate accurately since they require knowledge of optical models, level densities, and strength functions for the various possible exit channels. The objective of the Surrogate method is to determine or constrain these decay probabilities experimentally.

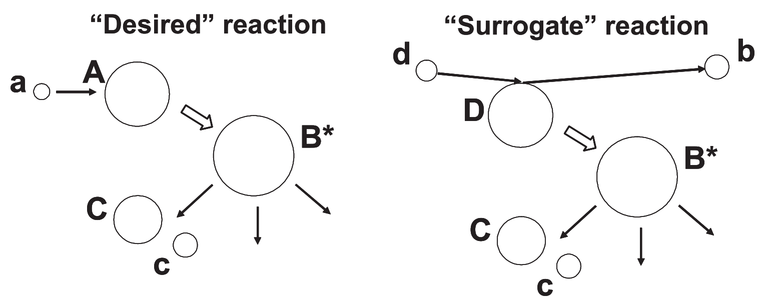

Figure 1: Schematic representation of the desired (left) and Surrogate (right) reaction mechanisms. The basic idea of the Surrogate approach is to replace the first step of the desired reaction, $a + A$, by an alternative (Surrogate) reaction, $d + D \to b + B^*$, that populates the same compound nucleus. The subsequent decay of the compound nucleus into the relevant channel, $c + C$, can then be measured and used to extract the desired cross section.

In the Surrogate approach, the compound nucleus B^* is produced by means of an alternative, direct (Surrogate) reaction, $d + D \to b + B^*$, and the desired decay channel $\chi(B^* \to c + C)$ is observed in coincidence with the outgoing particle b (see Figure 1). The coincidence measurement provides

$$P_{\delta\chi}(E_{ex}) = \sum_{J,\pi} F_\delta^{CN}(E_{ex}, J, \pi) \;\; G_\chi^{CN}(E_{ex}, J, \pi) \;, \tag{2}$$

the probability that the compound nucleus was formed in the Surrogate reaction with spin-parity distribution $F_\delta^{CN}(E_{ex}, J, \pi)$ and subsequently decayed into the channel χ.

The relevant information can be extracted from Surrogate experiments when either one of the following two conditions is met:

1. The spin-parity distributions in the decaying compound nucleus B^* are the same in the desired and Surrogate reactions, *i.e.* $f_\alpha^{CN}(E_{ex}, J, \pi) = F_\delta^{CN}(E_{ex}, J, \pi)$, where $f_\alpha^{CN}(E_{ex}, J, \pi) = \sigma_\alpha^{CN}(E_{ex}, J, \pi)/\sum_{J',\pi'} \sigma_\alpha^{CN}(E_{ex}, J', \pi')$ and $F_\delta^{CN}(E_{ex}, J, \pi)$ give the probabilities of producing states with spin J and parity π in the desired and Surrogate reactions, respectively.

2. The decay probabilities $G_\chi^{CN}(E_{ex}, J, \pi)$ are independent of $J\pi$, *i.e.* $G_\chi^{CN}(E_{ex}, J, \pi) = \mathcal{G}_\chi^{CN}(E_{ex})$.

In the first case, the measured coincidence probabilities of Equation 2 are proportional to the sought-after cross section, Eq. 1 and the proportionality factor can be calculated. However, since little is known about the spin-parity distributions in compound nuclei produced via direct reactions, it is not clear that the spin-parity distributions relevant to the desired reactions can be successfully reproduced in a Surrogate experiment. This approach would also be complicated by the fact that the $J\pi$ populations in both the desired and the Surrogate reaction are energy-dependent.

In the second case, the expression for the desired cross section simplifies to

$$\sigma_{\alpha\chi}^{WE}(E_a) \;\; = \;\; \sigma_{\alpha}^{CN}(E_{ex})\,\mathcal{G}_{\chi}^{CN}(E_{ex}) \tag{3}$$

where $\sigma_{\alpha}^{CN}(E_{ex}) = \sum_{J\pi} \sigma_{\alpha}^{CN}(E_{ex}, J, \pi)$ is the reaction cross section describing the formation of the compound nucleus at energy E_{ex} and $\mathcal{G}_{\chi}^{CN}(E_{ex})$ denotes the $J\pi$-independent branching ratio for the exit channel χ. This is the Weisskopf-Ewing limit of the Hauser-Feshbach theory [26, 17]. It provides a simple and powerful approximate way of calculating cross sections for compound-nucleus reactions. In the context of Surrogate reactions, it greatly simplifies the application of the method: It becomes straightforward to obtain the $J\pi$-independent branching ratios $\mathcal{G}_{\chi}^{CN}(E_{ex})$ from measurements of $P_{\delta\chi}(E_{ex})$ [$= \mathcal{G}_{\chi}^{CN}(E_{ex})$, since $\sum_{J\pi} F_{\delta}^{CN}(E_{ex}, J, \pi) = 1$] and to calculate the desired reaction cross section. Almost all applications of the Surrogate method to date have been carried out under the simplifying assumption that the Weisskopf-Ewing limit is applicable. Some of our findings regarding this assumption will be discussed in Section 3.2.

If neither condition 1 or 2 is met, a more comprehensive treatment of the Surrogate reaction becomes necessary in order to account for the so-called *spin-parity population mismatch*, the difference between the compound-nuclear spin-parity distributions that occur in the desired and Surrogate reactions, respectively: The distribution $F_{\delta}^{CN}(E_{ex}, J, \pi)$, associated with the Surrogate reaction, has to be determined theoretically, so that the branching ratios $G_{\chi}^{CN}(E_{ex}, J, \pi)$ can be extracted from the Surrogate measurements. In practice, the decay of the compound nucleus has to be modeled and the $G_{\chi}^{CN}(E_{ex}, J, \pi)$ have to be obtained by adjusting parameters in the model to reproduce the measured probabilities $P_{\delta\chi}(E_{ex})$ [41, 42]. Subsequently, the sought-after cross section is obtained by combining the calculated cross section $\sigma_{\alpha}^{CN}(E_{ex}, J, \pi)$ for the formation of B^* (from $a + A$) with the extracted decay probabilities $G_{\chi}^{CN}(E_{ex}, J, \pi)$ for this state, see Eq. 1.

This latter, more comprehensive treatment is typically not employed in Surrogate applications, since it requires significant theoretical input, including the theoretical prediction of the spin-parity population relevant to the Surrogate reaction. First steps towards predicting the spin-parity population of a compound nucleus produced in a direct reaction were taken by Andersen *et al.* [4], Back *et al.* [5], and, more recently, by Younes and Britt [41, 42]. These authors employed simple transfer calculations to estimate compound-nucleus spin-parity distribution following various stripping reactions on actinide targets. Younes and Britt used the resulting spin-parity distributions to re-analyze Surrogate (t,pf), (^{3}He,df), and (^{3}He,tf) fission-correlation measurements from the 1970s [15, 10] in order to extract (n,f) cross sections. Compared to earlier Surrogate analyses of the data, which were carried out assuming the validity of the Weisskopf-Ewing approximation, their estimated (n,f) cross sections showed significantly improved agreement with evaluated results, where available. Their findings underscored the importance of accounting for the spin-parity mismatch between the desired and Surrogate reactions and highlighted the need for further development of theories that describe the processes involved in forming a compound nucleus via a direct reaction. An important objective of the research pursued in this LDRD project has been to investigate the role of the spin-parity mismatch in other mass regions and for other Surrogate mechanisms, such as inelastic scattering and pickup reactions.

2 Research Goals and Activities

2.1 Goals of the project

The overarching goal of this LDRD project was to develop the theoretical and experimental framework for planning and analyzing Surrogate experiments that provide cross section information for reactions involving unstable targets. The work was focused on reaction mechanisms that are of interest to astrophysical applications and on mass regions containing nuclei that play a key role in the production of the heavy elements. Specifically, our work investigated the possibility of obtaining low-energy (n,γ) cross sections for s-process branch point nuclei in the mass 90-104 region and in the rare earth region. Apart from a couple of preliminary, unpublished studies [8, 9], there were no known Surrogate experiments in these mass regions. Furthermore, very little theoretical work had been carried out to investigate and address the challenges involved in extending Surrogate applications in these mass regions. We established the following research objectives:

- Identify and develop the theoretical models, codes, and related tools to investigate the crucial physics issues associated with Surrogate reactions.
- Examine the feasibility of applying the Surrogate method to reactions relevant to the astrophysical s process. This involved investigating the validity of the Surrogate approach for reaction processes, mass regions, and energy regimes that had not been studied previously.
- Study the validity of approximations to the full Surrogate formalism for applications of interest to astrophysics.
- Identify signatures and observables, as well as specific experiments, that can serve as tests for the theoretical developments, establish benchmarks for the Surrogate method, and provide additional insights into the Surrogate mechanisms.
- Carry out experiments that provide benchmarks for the Surrogate method.
- Upon successful completion of the benchmark experiments, carry out Surrogate experiments that allow for the determination of previously unknown cross sections.

Next, we provide a brief summary of our research activities during this LDRD project. Some of the findings resulting from our work will be discussed in Section 3. Additional achievements will be summarized in Section 4.

2.2 Outline of activities

In order to assess whether the Surrogate technique can be used to reliably determine the cross section for a particular desired reaction, various theoretical and experimental challenges have to be addressed. The most obvious issue that needs to be studied is the so-called *"J^π population mismatch"*: As outlined in the previous section, the Surrogate reaction populates the states in the intermediate nucleus differently than the desired $a + A$ channel, i.e. the weights $F_\delta^{CN}(E,J,\pi)$ by which the decay probabilites $G_\chi^{CN}(E,J,\pi)$ are multiplied in equation (2), are different from the formation probabilities $\sigma_\alpha^{CN}(E,J,\pi)/\sum_{J',\pi'}\sigma_\alpha^{CN}(E,J',\pi')$ of equation (1), and depend on the direct reaction under consideration. In the early work it was assumed that the experimental conditions were such that the Weisskopf-Ewing limit applied. More recent work by Younes and Britt, which employed a simple model to account for the spin-parity mismatch in stripping reactions, demonstrated the importance of accounting for the J^π population mismatch in (n,f) reactions for Uranium targets [41, 42]. In the framework of the LDRD project, we developed models, codes, and tools that allow us to investigate the effect of the $J\pi$ population mismatch. We applied these tools to (n,γ) reactions involving spherical as well as deformed targets in mass regions relevant to the s process.

In order to test the limitations of the Weisskopf-Ewing approximation and to identify reactions that can possibly serve as Surrogates for a particular desired reaction, it is important to know the J^π populations that are obtained in various direct reactions (stripping, pick-up, inelastic scattering), as well as the dependence of these populations on projectile, target, excitation energy, angle of outgoing particle, etc. This is a nontrivial task since a proper treatment of direct reactions leading to highly excited states in the intermediate nucleus involves a description of particle transfers, and inelastic scattering, to unbound states. Younes and Britt considered stripping reactions only, and used a simple direct-reaction model. In the context of the LDRD work, we studied inelastic scattering with alpha particles from spherical targets, and (^{3}He,α) pickup reactions from deformed targets; see Section 3.5 and Section 3.6.

It is furthermore important to study how the J^π populations that can be obtained in the various reactions affect the *decay of a compound nucleus*. More specifically, if there is a significant J^π population mismatch between the Surrogate and desired reactions, one has to investigate whether the Surrogate measurement can provide meaningful constraints for the cross section of the desired reaction. We carried out calculations that addressed this issue for zirconium nuclei. We identified the primary challenges involved in obtaining (n,γ) cross sections for target nuclei near closed shells and demonstrated the limitations of commonly-employed approximate methods. We also identified strategies for obtaining valuable cross section information under such adverse circumstances. Our findings, which have been submitted for publication, are briefly summarized in Sections 3.1, 3.2, and 3.3.

A proper investigation of the issues outlined above necessitates experiments that test the theoretical developments, establish benchmarks and provide additional insights. Experimental work, partially supported by LDRD funds, was carried out by Livermore scientists, in collaboration with researchers from Lawrence Berkeley National Laboratory, the University of Richmond, and Yale University. Several new experiments were developed and carried out during the LDRD funding period. The analyses of these new Surrogate experiments presented challenges that required new techniques to be developed. Details are given in Section 3.8.

Additional activities: Apart from technical work carried out in the framework of this LDRD project, efforts were made to increase awareness of the issues related to the Surrogate approach in the basic science community and to form collaborations with researchers at other institutions in order to address the challenges involved. A workshop was organized (see Section 4.3), the Surrogate technique was presented at various international meetings (see Section 4.4), and several new collaborative efforts are now underway (see Section 4.1).

2.3 Research team and budget

The core research team involved in the "Surrogate Nuclear Reactions Project" was comprised of both nuclear theorists and experimentalists from N Division. More specifically, the project brought together expertise in Nuclear Structure and Reaction Theory (Jutta Escher, Frank Dietrich, Christian Forssén, and Vesselin Gueorguiev), Nuclear Astrophysics (Rob Hoffman), and Experimental Nuclear Physics (Larry Ahle, Lee Bernstein, Jason Burke, and Jennifer Church). Darren Bleuel, an experimental postdoc from LBNL (now a postdoc at LLNL) joined our effort in the spring of 2006. During the course of the project we closely collaborated with experimentalists from Yale University, the University of Richmond, and Berkeley National Laboratory and we benefited from the expertise of various reaction theorists who have close ties to the Nuclear Theory and Modeling (NT&M) Group. In particular, we initiated interactions with Prof. Ian Thompson from the University of Surrey, UK, who subsequently joined the NT&M Group in the context of a strategic hire.

Throughout the course of the project, LDRD funding provided for approximately 50% of the salary of the PI, the full salary of a theory postdoc (one-half for C. Forssén and V. Gueorguiev each), 50% of the salary of an experimental postdoc, and some travel and incidental costs. The budget received was $280k in FY04, $281.5k in FY05, and $280k in FY06 (the latter number was later adjusted to $383k to cover increased overhead rates).

2.4 Impact of budget cuts in FY06

Funding in the final year reflects a 20% cut that was applied across all LDRD-ER projects during that year. This budget cut had adverse and very unfortunate effects on the research project. We were in the process of replacing Jennifer Church, who had been promoted from a postdoctoral position to a staff position when the budget cuts and associated hiring slown-down occured. As a result, we were not able to extend an offer in a timely manner to the person whom we had identified as the replacement postdoc, who lived already in the Bay area and who was ready to start working on Surrogate experiments. Shortly before that, Dr. Church had moved from working full-time on Surrogate experiments to dedicating almost all her time to another project and we were left for more than six months without a postdoc dedicated to the planning, execution, and analysis of additional experiments. It took until late-February of 2006 to find an alternate replacement: Dr. Darren Bleuel was fortunately already somewhat familiar with the experimental facilities at LBNL and did not have to relocate to start working with our team. As a result of the reduced funding and associated delays, we had to cancel one of the two experiments that were planned for FY06. Furthermore, we were not able to finalize the analysis and interpretation of the one experiment that did take place in FY06. This work is now being pursued with other funds. Dr. Bleuel's progress to date is summarized in Section 3.8. Due to the budget cuts and necessary re-arrangements of the tasks associated with this, we also had to eliminate the theoretical investigation of the role of non-equilibrium decays in Surrogate reactions, that was planned for FY06.

3 Research results and insights

The theoretical and experimental research carried out in the context of this LDRD project has resulted in new insights and developments that are valuable for current and future applications of the Surrogate approach. In particular, the past three years have seen the following accomplishments:

1. We have developed models (and associated codes and tools) that provide insights into the formation of a compound nucleus in a Surrogate reaction. Our work has focused on inelastic scattering from spherical and near-spherical targets. Inelastic scattering to highly-excited states above the particle-emission threshold, which had received very little attention prior to our work, can be especially valuable for Surrogate applications to s-process branch points. We also investigated pickup reactions for deformed targets.

2. We have identified and begun to implement additional developments that will extend our work beyond the goals of the LDRD project, further our understanding of the mechanisms present in a Surrogate reaction and improve the reliability of cross sections extracted from Surrogate experiments.

3. We have achieved a much improved understanding of the applicability and limitations of the Weisskopf-Ewing approximation in Surrogate reactions.

4. We have demonstrated how uncertainties in the theoretical models that are employed to interpret Surrogate experiments affect the cross sections extracted from the data.

5. We have identified and illustrated with calculations the challenges associated with extracting (n,γ) cross sections for near-spherical target nuclei. We have also identified methods for obtaining valuable cross section information for such challenging situations.

6. We formulated suggestions and recommendations for carrying out experiments that can test the theoretical developments, provide insights into the Surrogate reaction mechanisms, and establish benchmarks for the method.

7. We have developed and improved the experimental apparatus, tools and techniques necessary for carrying out Surrogate experiments. We have developed new tools for analyzing Surrogate data.

8. We have carried out experiments that were selected as valuable benchmark experiments for the Surrogate method.

9. We have identified challenges that particularly affect Surrogate experiments aiming at extracting low-energy (n,γ) cross sections for astrophysical applications. We have outlined strategies for addressing these issues in future experiments.

Below, we briefly highlight our main technical results and basic science findings. Additional, related accomplishments (publications and presentations, training and recruiting, collaboration-building efforts, workshop organization, etc.) are summarized in Section 4.

3.1 General insights regarding Surrogate applications to reactions relevant to the astrophysical s-process

As explained in Section 1.1, improved nuclear reaction cross sections are required to test available s-process models, to provide information on the physical conditions under which the process takes place, and to impose constraints for the less well-known r process. Of particular interest are s-process branch points, unstable nuclei that are produced in the s process with a life time long enough to allow the s process to proceed by either neutron capture or beta decay [29]. Accurate neutron capture cross sections for branch-point nuclei such as ^{85}Kr, ^{95}Zr, ^{153}Gd, ^{151}Sm, etc. are required to understand various interesting astrophysical phenomena. Capture cross sections for several Zr isotopes (A=90, 91, 92, 93, and 96), as well as the ^{151}Sm(n,γ) cross section have recently been measured directly [3]. Direct measurements of the cross sections for other compound-nuclear reactions, such as the ^{85}Kr(n,γ), ^{95}Zr(n,γ), and ^{153}Gd(n,γ), remain challenging. Since calculated capture cross-sections are often very uncertain [6], it is worthwhile to investigate whether the Surrogate approach can provide additional information. The compound nuclei relevant to the above cases, ^{86}Kr*, ^{96}Zr*, and ^{154}Gd*, can be obtained, e.g., via inelastic scattering on ^{86}Kr and ^{96}Zr in the first two cases, and a one-neutron pickup reaction, e.g. (^{3}He,α), on ^{155}Gd in the latter case. In some sense, s-process branch points provide an excellent opportunity for Surrogate applications. The desired reaction is a neutron-capture reaction on an unstable nucleus ^{A}Z which is located very close to the valley of stability. Often, both its ^{A-1}Z neighbor and the intermediate nucleus ^{A+1}Z that is formed in the neutron-capture process are long-lived. Consequently, there are various options for forming the relevant compound nucleus in a Surrogate (direct) reaction, e.g. via a 2-neutron pickup reaction on ^{A-1}Z or inelastic scattering on ^{A+1}Z. On the other hand, the neutron energies relevant to the s process are very low. Current s-process scenarios have characteristic temperatures corresponding to neutron energies $E_n =$ 8 and 23 keV for the production of the elements between Zr and Bi in the main s-process component, and $E_n = 26$ and 91 keV for the production of the elements between Fe and Zr in the weak s-process component [29]. The low energies imply that very little angular momentum is transferred from the neutron to the target, while the angular-momentum transfer in the Surrogate reaction can be much larger, thus leading to significant differences between the compound-nucleus populations obtained in the two different reactions (see *spin-parity population mismatch* in Section 1.2).

3.2 Low-energy (n,γ) reactions on spherical targets and the limitations of the Weisskopf-Ewing approximation

The spin-parity population mismatch provides a major challenge for Surrogate applications to nuclei near closed shells, as can be inferred from the ^{91}Zr(n,γ) example presented in Figure 2. Shown is the probability that a ^{92}Zr state with excitation energy $E_{ex} = S_n + \varepsilon_n$ and given $J\pi$ value decays via γ-emission. For details of our calculation, see Ref. [25]. For neutron energies below about 2.5 MeV, the gamma decay probabilities depend very sensitively on angular momentum and parity. In this energy region, the decay of the ^{92}Zr compound nucleus proceeds exclusively by gamma or neutron emission. Due to the low level density in the neighboring ^{91}Zr nucleus, only a very small number of neutron decay channels are open. This circumstance, and the fact that the neutron transmission coefficients are very large for the s and p wave channels, and small for all other channels, leads to gamma-decay probabilities that are very sensitive to the $J\pi$ population of the decaying compound state. It is clear that the Weisskopf-Ewing approximation is not valid in this region. With increasing energy, more levels in ^{91}Zr become available and the dependence of the decay probabilities on angular momentum and parity becomes weaker. The situation is also expected to improve as one moves away from closed-shell nuclei. For example, while ^{91}Zr has only one level below 1 MeV (the ground state), ^{101}Ru has more than ten, and ^{155}Gd has over 60. Consequently, the decay probabilities for ^{102}Ru and ^{156}Gd can be expected to depend more smoothly on energy and to exhibit less sensitivity to the $J\pi$ values of the compound nucleus.

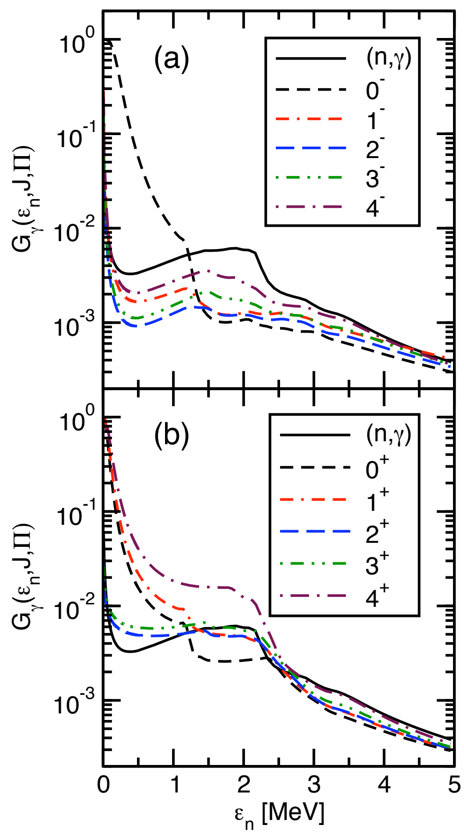

Figure 2: Gamma branching ratios as a function of spin, parity and excitation energy of the decaying state in ^{92}Zr. The energy is given as the equivalent neutron energy $\varepsilon_n = E_{ex} - S_n$. For reference purposes, the total gamma-decay probability following neutron absorption is shown as a solid line in both panels.

3.3 Challenges associated with spherical s-process branch points and possible solutions

The fact that the ^{91}Zr(n,γ) reaction involves a target very near a closed shell makes this reaction a particularly difficult candidate for a Surrogate treatment. For energies below 2.5 MeV, the Weisskopf-Ewing approximation cannot be employed and the accuracy of the cross section obtained from a full Surrogate analysis will be limited, since small errors in the predicted Surrogate $J\pi$ population $F_{\delta}^{CN}(E, J, \pi)$ introduce large uncertainties in the extracted decay probabilities. For details about the sensitive dependence of the extracted cross sectin on small errors in $F_{\delta}^{CN}(E, J, \pi)$, see Ref. [25]. However, even in this extreme case, it may be possible to obtain some useful reaction information from a Surrogate experiment. Since Surrogate experiments can provide coincidence probabilities $P_{\delta\chi}(E)$ for a wide range of energies, one can study a region for which the Weisskopf-Ewing limit is approximately valid ($E_n > 2.5$ MeV in the current example) and use the results to normalize the calculated decay probabilities. The deduced normalization factor can subsequently be used in the statistical reaction calculation of the cross section in the desired energy range. This approach was tested with the help of statistical nuclear-reaction simulations [25]. The bottom panel of figure 3 demonstrates that the cross sections obtained in this approach agree well with the expected result (solid black line). The colored (broken) curves represent three different simulations that illustrate the effects of the two major uncertainties inherent in the Surrogate method: (i) Insufficient knowledge of the decay pattern for the relevant compound nucleus, which must be supplemented by reaction modeling; (ii) Insufficient knowledge of the spin-parity distribution of the decaying compound nucleus. The normalization approach appears to be quite robust and affected little by these uncertainties. For more details, see Ref. [25]. Since the ^{91}Zr(n,γ) reaction discussed here represents an especially challenging example, we expect our normalization approach to work equally well or better in other situations where the Weisskopf-Ewing approximation is not valid.

3.4 General insights regarding the prediction of compound-nucleus spin-parity distributions in Surrogate reactions

Predicting the spin-parity distribution for a compound nucleus produced in a Surrogate reaction requires a careful consideration of the reaction mechanisms that are involved in the formation of the compound nucleus. In the absence of width fluctuation corrections, the challenge of describing the relevant reaction mechanisms can be divided into two separate problems:

1) the formation of a highly-excited nucleus in a direct reaction, and

2) the damping of the excited states into the compound nucleus.

Incorporating width fluctuation correlations will introduce additional complications.

Addressing the first problem necessitates developing a quantitative description of the direct-reaction process that allows for a prediction of the spin-parity distribution in the highly-excited intermediate nucleus, immediately following the direct reaction. Such a description is also nontrivial since it requires a framework for calculating cross sections of

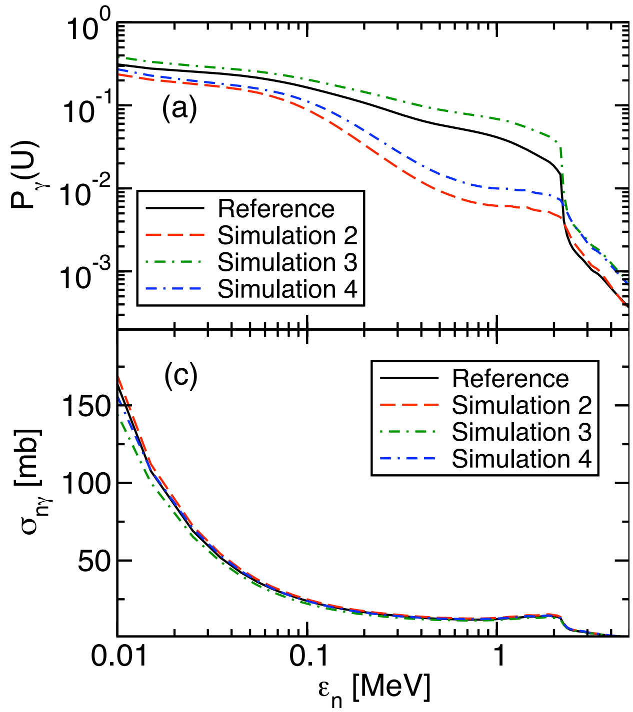

Figure 3: (top) Gamma-decay probabilities for different simulations. The solid line corresponds to the reference decay probability while the three other curves are based on calculations that simulate the effects of uncertainties inherent in the Surrogate approach. (bottom) The extracted cross sections, for the respective simulations, obtained by employing the normalization approach. The results agree well with the expected, reference, cross section (solid line) and exhibit little sensitivity to uncertainties in the modeling. Note that $E = \varepsilon_n + S_n$.

different reactions (stripping, pick-up, and inelastic scattering) to continuum states, for a variety of projectiles (p, d, t, α, etc.) and targets (spherical as well as deformed).

The second problem is associated with the subsequent evolution of the intermediate nucleus. The assumption that a compound (i.e. equilibrated) nucleus is formed is central to the Surrogate method. Rapid decay of the intermediate configuration before a compound nucleus can be formed would invalidate the Surrogate analysis. The competition between particle emission and equilibration, and its dependence on the spin and parity of the intermediate nucleus, needs to be investigated[1].

Correlations between the incident and outgoing reaction channels affect in principle both the desired and Surrogate reactions. For the desired reaction, these correlations can be taken into account formally by including an additional (width fluctuation correction) factor in Equation 1 [26], while a similar simple solution is not readily available for the Hauser-Feshbach-type expression describing the Surrogate reaction, Eq. 2. An examination of the

[1]This process should not be confused with pre-equilibrium emission of particles in the desired reaction, $a + A \rightarrow c + C$; contributions from the latter cannot be determined via the Surrogate approach and need to be calculated separately and added to the desired cross section.

role of width fluctuation correlations was not part of this LDRD project, but should be included in an extended investigation of the formalism associated with the Surrogate approach.

Next, we will present results that address the first of the challenges outlined above. While we had originally expected to carry out a study of the second issue, the damping of the excited states into the compound nucleus, for (d,p) reactions, using methods developed by Dietrich and Kerman [30, 33], we had to cancel this research activity due to budget cuts in the last year of the LDRD project (see Section 2.4). We have, however, submitted a proposal to the Department of Energy's Office of Science to investigate this topic, as well as to explore the role of width fluctuation correlations.

3.5 Compound-nuclear spin-parity distributions following inelastic scattering with α particles

Inelastic scattering is an important direct-reaction mechanism for the Surrogate method, in particular for applications to reactions involving s-process branch points. Neutron-induced reactions on an s-process branch point ^{A}Z produce compound nuclear states in an isotope ^{A+1}Z with a ground state that is, by definition, much longer lived than the branch-point isotope, $t_{1/2}(^{A+1}Z) \gg t_{1/2}(^{A}Z)$. Hence, the best opportunity for producing the compound nucleus of interest may involve inelastic scattering off the ground state of ^{A+1}Z. The potentially very important role of inelastic scattering for such applications, plus the fact that little was known about inelastic scattering to highly-excited states above the particle-emission threshold motivated our work in this area. Recent experiments at LBNL involving α particles as projectile and the copious amounts of structure and reaction information available for ^{90}Zr guided our selection of ^{90}Zr(α,α')^{90}Zr* as the reaction to investigate in detail.

We developed a model to predict the spin-parity distribution in a compound nucleus produced via inelastic α scattering. Our focus was on obtaining a first, simple description of the direct-reaction process and on providing the basis for a more complete treatment of the problem. Our work, summarized in a technical report [20], identifies what a rigorous treatment of the mechanisms that produce a compound nucleus entails, specifies the approximations made in the present description, and provides details about the model and model inputs employed.

The model we developed is based on the assumption that the inelastic scattering cross section for ^{90}Zr(α,α')^{90}Zr* can be approximately expressed in terms of cross sections for producing uncorrelated particle-hole excitations in the target nucleus. Specifically, the cross section is given as an incoherent sum of scattering cross sections $(\frac{d\sigma}{d\Omega})_{m_h,m_p}$ for individual particle-hole excitations (m_h, m_p) with weights $|a(m_h, m_p)|^2$ that depend on the energy and spreading widths of the particle-hole configurations[2]. In Figure 4, we show the distribution of the neutron and proton particle-hole excitations generated in the model across an energy range of $E = 5-23$ MeV for the target nucleus ^{90}Zr* and illustrate the effect of the spreading. Inelastic scattering cross sections were calculated for each individual particle-hole excitation using the distorted-wave Born-approximation (DWBA).

[2]The spreading (or damping) widths Γ_{m_h,m_p} of the particle-hole excitations arise from their coupling to more complicated (2p-2h, etc.) configurations. It is this coupling that is driving the eventual formation of a compound nucleus. For practical applications, several analytic expressions, based on some underlying

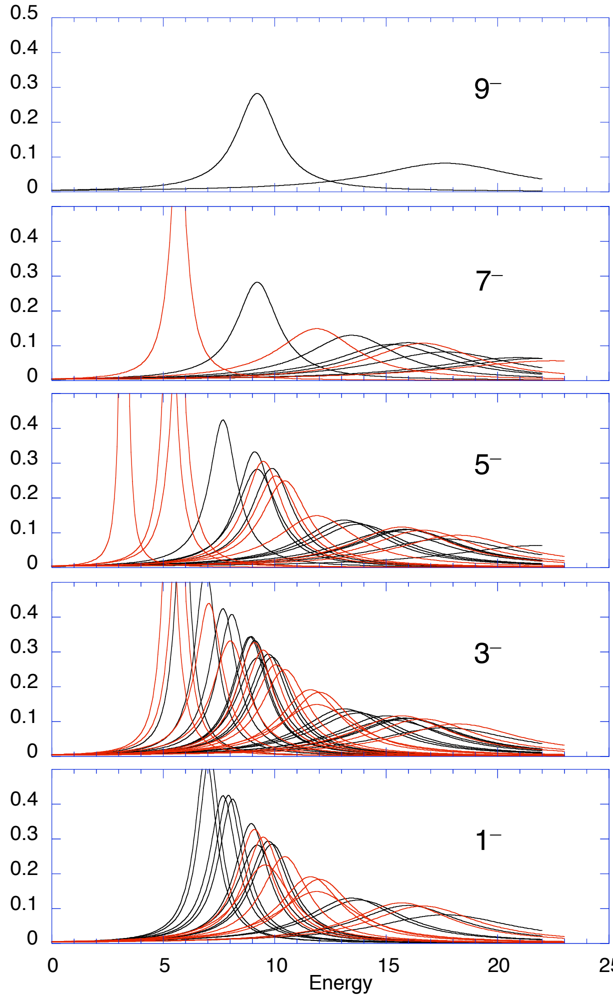

Figure 4: "Smeared" energy distributions of negative-parity particle-hole excitations in ^{90}Zr. Shown are Lorentzian shapes which approximate the energy spreading of particle-hole states due to residual many-body effects. All negative-parity states with $E > 5.0$ MeV are shown. Neutron (proton) particle-hole states are given in black (red) and the total angular momentum of the excited ^{90}Zr final state is indicated on the right side of the figure. Positive-parity excitations (not shown) exhibit a similar structure.

Combining the energy distributions of the particle-hole states shown in Figure 4 and the cross sections for the individual particle-hole excitations (not shown, see Ref. [20]) allowed us to determine the ^{90}Zr(α,α')^{90}Zr* scattering cross section as a function of the angle of the outgoing α particle, see Figure 5. Cross sections can be obtained for producing the excited ^{90}Zr nucleus at a particular excitation energy and for specified values of angular momentum and parity. The sum of the partial cross sections for different $J\pi$ values gives the total inelastic scattering cross section. While it is rare to find measured angular distributions for inelastic scattering reactions that produce nuclei above the particle emission threshold, data for inelastic α scattering experiments do exist for ^{90}Zr [40] and are compared to our calculations, see Figure 5. For angles in the range of 50° to 90°, we find that the calculated total scattering cross section is in good agreement with the data, while the calculations underestimate the cross section at forward angles by a factor on the order of 5. Note that no error bars were given for the experimental results. This level of agreement is not unreasonable for a model that describes the highly-excited ^{90}Zr nucleus in terms of uncorrelated particle-hole excitations. Including many-body correlations, in particular collective effects, will provide a more realistic picture of the scattering process and is expected to improve the agreement. Investigations into these effects have been initiated, see Section 3.6 below.

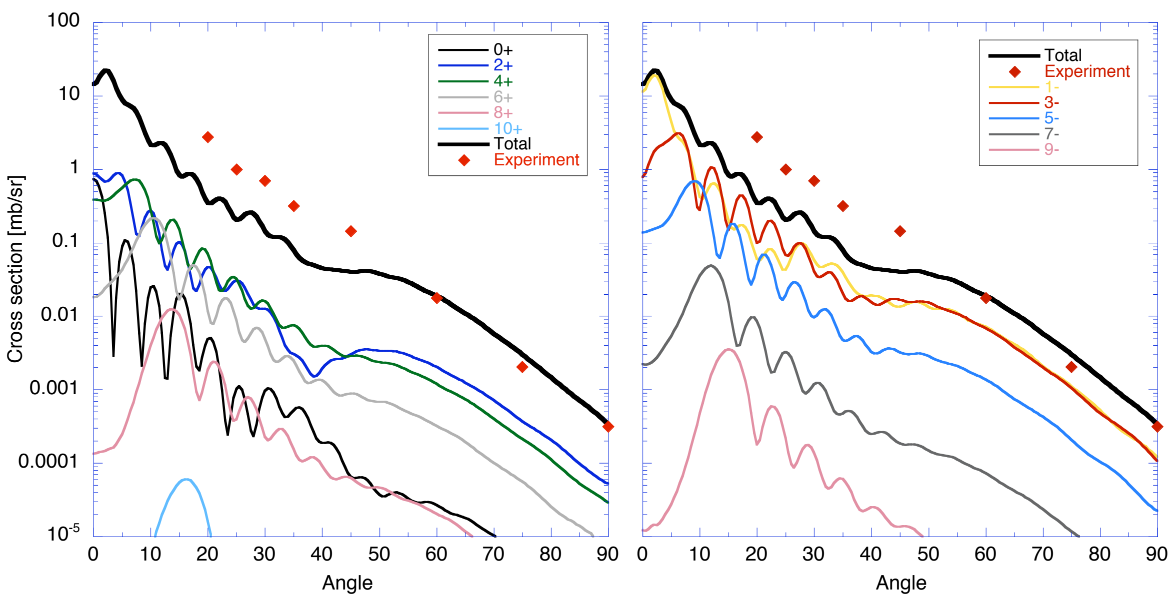

Figure 5: Inelastic scattering cross section for ^{90}Zr$(\alpha,\alpha')^{90}$Zr* with E_α=140 MeV and E'_α=130 MeV. The total scattering cross section (solid black line) is compared to experimental results. Also shown are the contributions to the scattering cross section that lead to various $J\pi$ states in ^{90}Zr*. Contributions from positive (negative) states are shown on the left (right).

theoretical approach and developed to reproduce empirical results, can be found in the literature.

A prediction for the compound-nucleus spin-parity distributions produced via inelastic scattering can be obtained from the calculations described above. The probablilties for populating different $J\pi$ states are shown in a linear plot in Figure 6, as a function of the scattering angle. The distance between two adjacent curves gives the probability of finding the spin and parity indicated by the values listed at the right end of the upper curve. For example, at 90°, we find about 0% contribution from 0^+ states, 15% from 2^+ states, 8% from 4^+ states, etc. The left panel gives the probabilities obtained by dividing the cross sections for the various $J\pi$ values by the total inelastic scattering cross section. The right panel shows a probabilities that have been smoothed in order to account for experimental uncertainties and "binning" in the angular measurements. We observe that the $J\pi$ distribution is, as expected, angle-dependent, with the largest uncertainties occurring at forward angles ($< 40°$). At larger angles, the probabilities are less sensitive to the angle of the outgoing α particle. Knowing the angular-momentum and parity populations is important for the planning and analysis of Surrogate experiments, since these distributions determine the weights $F(E, J, \pi)$ for the decay probabilities $G_\chi(E, J, \pi)$ that are to be determined or constraint via a measurement of $P_{\delta\chi}$ (see Equation 2). The results shown here are for excitation energy $E_{ex} = 10$ MeV; it is straightforward to generate results for other energies [20].

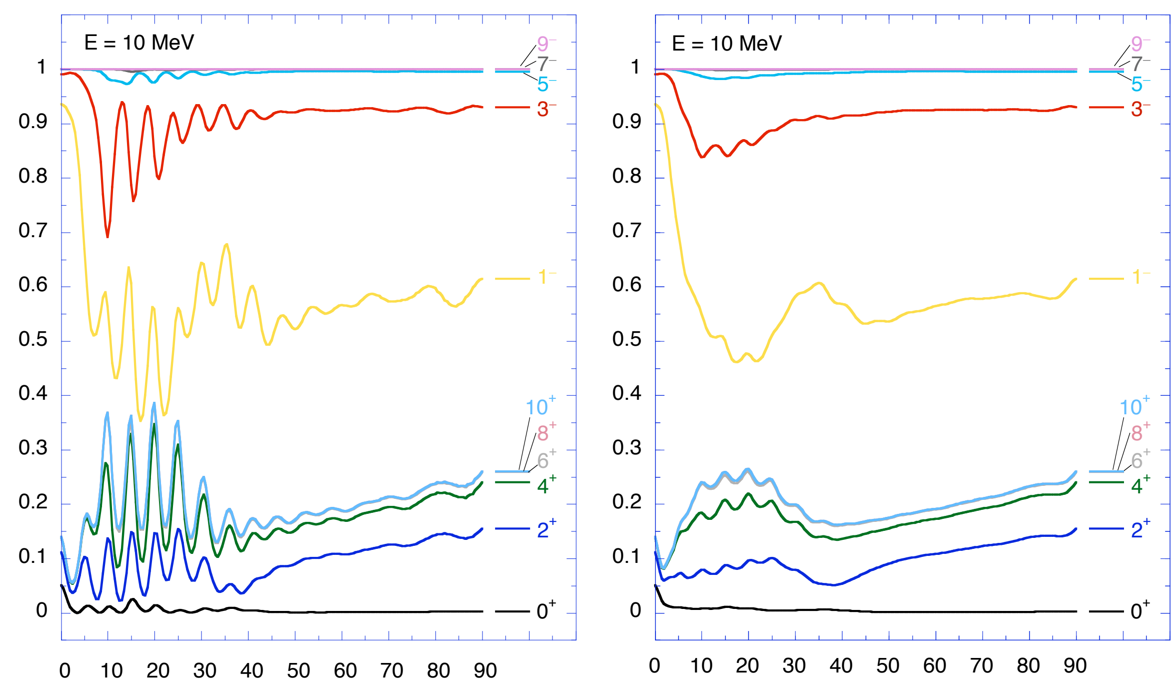

Figure 6: Probabilities for populating various $J\pi$ states in $^{90}Zr^*$ following inelastic alpha scattering with 140 MeV projectiles that leave the target nucleus at excitation energy E_{ex} =10 MeV. The left panel shows the results of the calculation, the right panel shows probabilities that have been smoothed in order to account for experimental uncertainties and "binning" in the angular measurements.

3.6 Extension of the inelastic scattering treatment to include collectivity

It is likely that a simple single-particle picture is adequate to describe the spectroscopy of the nuclear configurations reached immediately following a direct reaction of the stripping or pickup reaction type (e.g. (^{3}He,α)) at high excitation energies relevant to Surrogate reactions. However, exciting the nucleus by inelastic scattering (e.g. (p,p) or (α,α)) may require a more detailed picture since this type of reaction is highly sensitive to nuclear collectivity. These effects are not included in the uncorrelated particle-hole model that serves as the simplest picture of the spectroscopy required for inelastic scattering. Under this LDRD project we have developed a framework and implemented computer codes to study the effects of collectivity and to compare the results with those obtained with the uncorrelated particle-hole model, described in Section 3.5. The description of the formalism has been written up as a technical report [18]. The calculations are carried out by constructing the transition densities for every relevant state in the desired excitation-energy range (roughly 5-30 MeV), and then convoluting the transition density with an effective interaction between the projectile and target nucleus to yield a transition potential. This transition potential is then used as input to a distorted-wave Born-approximation (DWBA) code to calculate angular distributions and cross sections for the scattered projectile. The transition densities are constructed using single-particle wave functions obtained from a nuclear Hartree-Fock code. These wave functions are sufficient to calculate transition densities in the uncorrelated particle-hole model. To include collectivity, we use the random-phase approximation (RPA) to provide the appropriate correlations. Both the Hartree-Fock and RPA calculations use codes developed at Bruyères-le-Châtel by Dr. Daniel Gogny, and the work is being carried out in collaboration with Dr. Daniel Gogny (now at LLNL) and Dr. Marc DuPuis (now at LANL). First tests of these procedures have been carried out for an uncorrelated particle-hole transition.

We are currently extending our investigations beyond the original goals of the LDRD project: We are applying the techniques described above to inelastic alpha scattering on ^{90}Zr and will use this reaction as a test case to determine whether the inclusion of collectivity significantly modifies the spin-parity distribution in the residual nucleus from that obtained in the uncorrelated particle-hole approximation. If so, the RPA technique should be applied whenever inelastic scattering is used in a Surrogate-reaction experiment, and further investigations, including an extension to deformed nuclei, should be carried out if funding is available to do so. We expect to submit these results for publication in a scientific journal, since to our knowledge there are no equivalent comparisons of mechanisms for inelastic scattering to highly-excited states.

3.7 Transfer reactions on deformed targets and compound-nuclear spin-parity distributions

Since many s-process branch point nuclei are deformed, developing theoretical descriptions for Surrogate reactions on deformed nuclei becomes important. We began our theoretical development with an investigation of pickup reactions in the rare-earth region. Specific applications of interest include (^{3}He,α) reactions on Gd targets. Surrogate experiments of that type were carried out at LBNL with the goal to extract (n,γ) cross sections that can be compared to available, directly-measured results (see Section 3.8 below). In addition, ^{155}Gd(^{3}He,α)^{154}Gd produces the compound nucleus ^{154}Gd that is relevant to the radiative capture reaction ^{153}Gd(n,γ) on the important s-process branch point ^{153}Gd.

We employed and expanded a method introduced by Andersen *et al.* [4] for the calculation of single-particle form factors and corresponding energies in a deformed potential. The distorted-wave Born-approximation (DWBA) approach was then used to obtain the cross sections for pickup from deformed, deeply-bound states in Gadolinium nuclei (see Ref. [27]. An alternative approach, based on a coupled-channels formalism, was recently developed by Thompson *et al.* [38], who applied the method to actinide nuclei. A careful comparison of the two methods will serve as a validation of both approaches and will provide further insights into the validity of some of the approximations employed in the two different approaches. The resulting spin-parity distributions will be, upon verification, employed to complete the interpretation of the ^{157}Gd(^{3}He,α)^{156}Gd experiment that aims at extracting the known ^{153}Gd(n,γ) cross section and that is currently being analyzed by Dr. Bleuel (see Section 3.8 below). The insights gained from the theoretical predictions and from the results of this experiment will also serve as a basis for planning an additional Surrogate experiment that allows for the determination of the ^{153}Gd(n,γ) cross section.

3.8 Surrogate experiments in the rare-earth region

In May 2006 a Surrogate experiment was performed using the STARS+LIBERACE set-up at the 88-Inch cyclotron at LBNL. The purpose of this experiment was to investigate the validity of the Surrogate technique to obtain (n,γ) cross sections at astrophysically relevant energies in a deformed rare earth nucleus. Despite the negative impact of the FY06 budget cuts on this particular experimental activity (one of the two planned experiments had to be cancelled and the analysis of the other was significantly delayed due to hiring issues associated with budget issues – see Section 2.4), some significant progress was made towards examining the possibility of applying the Surrogate method in the rare-earth region.

The (desired) reaction to be investigated was ^{155}Gd(n,γ). This reaction was chosen due to the copious amount of data available for neutron energies below 1 MeV and for the ability to populate the relevant compound nucleus, ^{156}Gd, via the Surrogate ^{157}Gd(^{3}He,α)^{156}Gd reaction. The (^{3}He,^{3}He) data was studied in addition to the (^{3}He,α) data. The data analysis from this experiment was performed by a LBNL post-doctoral researcher, Dr. Darren Bleuel (now at LLNL), and has been presented at the APS/DNP 2006 meeting in Nashville, TN.

The analysis of this data provided detailed insight into the issues involved in tagging a specific exit channel probability for the Surrogate method using discrete low-lying γ-rays in the residual nucleus. The major issues associated with such measurements are: 1) Determining the total number of outgoing particles from reactions on the target of interest and differentiating these particles from reactions on Oxygen and Carbon contaminants on the target. 2) Quantifying any energy dependence in the response of the detector array to both particles and γ-rays. The latter task is significantly harder than the former. 3) Determining the efficiency with which the residual nucleus can be determined. This efficiency is influenced by both experimental and modeling factors including the total particle-γ coincident efficiency of the STARS+LIBERACE array and the probability with which a given low-lying transition is populated in the residual nucleus.

A number of steps were taken to address the issues listed above under heading 1). A detailed analysis of both ^{3}He and α particle singles spectra was performed by Dr. Bleuel. He determined that there was significant contamination from ^{16}O on the target. This caused an uncertainty in the total particle number at energies at and below the elastic scattering energy. However, Dr. Bleuel also determined that there were several energy regions where the particle spectrum was clear of contamination and an absolute Surrogate measurement could be performed.

As a part of this analysis Dr. Bleuel also gained significant insight into the performance of STARS as a function of the energy of the outgoing particle (issue 2 above). Dr. Bleuel was the first member of the collaboration to notice that there was significant cross-talk at high energies between adjacent rings and sectors in the particle detectors. It was determined that this cross-talk was present in all experimental data where the Silicon detectors were over-biased to enhance their energy resolution. Once this cross-talk was quantified algorithms were developed to remove the cross-talk effects from the particle data and allow further analysis. Unfortunately, these algorithms may have introduced significant changes in the overall particle detection efficiency at low excitation energies. This issue will be addressed in greater detail below.

Dr. Bleuel also focused significant effort on determining the efficiency with which the exit channel could be tagged using discrete γ-rays. This efficiency was first determined using the technique set forth in Bernstein et al. [7], where the intensities of γ-rays from ^{156}Gd were determined for particle energies corresponding to excitation energies where the only decay path for the ^{156}Gd nucleus was via γ-rays. At these energies the total number of γ-rays observed divided by the total number of particles observed is equivalent to the ability to tag the formation of a ^{156}Gd residual nucleus using that specific γ-ray. The resulting efficiency was then compared to the absolute particle-γ efficiency obtained by looking at discrete γ-rays from particle-γ-γ coincident data from the ground state band of ^{156}Gd. The results from these two different approaches yielded similar results lending further credence to the tagging efficiency determined using the approach listed in [7].

The results obtained to-date from Dr. Bleuel's analysis were presented at the APS/DNP 2006 meeting in Nashville TN. In short, the (n,γ) cross section estimate obtained (using the Weisskopf-Ewing approximation) was similar in shape to the one previously determined directly, but the absolute magnitude differed by a factor of approximately 2. Similar results were obtained for the ^{155}Gd(n,2n) and the Surrogate ^{157}Gd(^{3}He,α2nγ) cross sections. In order to explain the discrepancy between the ^{155}Gd(n,γ) cross section that was directly measured and the one extracted from our Surrogate experiment, additional work is needed. In particular, the possibility that the algorithm used to correct for the cross-talk between adjacent channels introduced an energy-dependent skew on the particle data needs to be investigated. Furthermore, the effects of the $J\pi$ mismatch have to be explored and accounted for in the interpretation of the data. This latter effort will make use of the theoretical tools developed in connection with the LDRD project.

The experimental goals that were pursued in the context of the LDRD project (see Section 2.1) are still important objectives for any experimental effort in the area of Surrogate reactions. In fact, an additional experiment was carried out in October 2006 to explore whether a variant of the Surrogate approach described here, the Surrogate Ratio

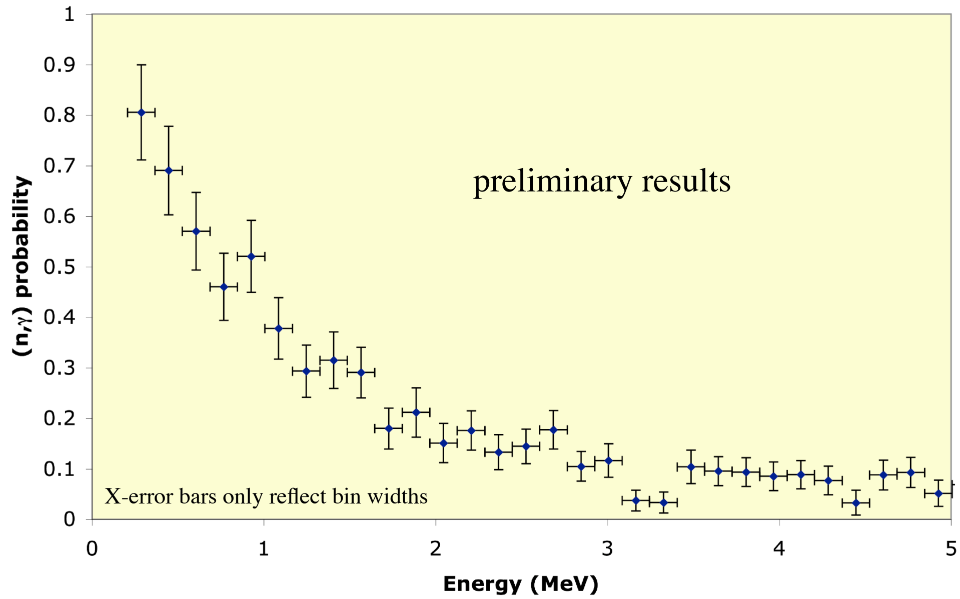

Figure 7: Branching ratio of ^{156}Gd(n,γ) calculated via the absolute Surrogate method, based on the 199 keV $4^+ \rightarrow 2^+$ transition observed in ^{157}Gd(^{3}He,α) reactions. While the general shape is correct, when multiplied by the total neutron cross section, the magnitude is about twice the published (n,γ) cross-section. Efforts are ongoing to determine if this is due to issues with the data analysis and collection or an indication of the limitation of the absolute Surrogate method.

method [34, 12, 7, 21, 22] can be employed to determine (n,γ) cross sections for the deformed rare-earth isotopes ^{171}Yb and ^{173}Yb. Preliminary results from this experiment were presented at the APS/DNP 2006 meeting and at the SSAAP07 symposium in Washington DC. In addition, a new experiment is planned to determine several Gadolinium (n,γ) cross sections using both the absolute and Surrogate Ratio methods. This experiment, which will employ lower energy inelastic proton scattering in order to maximize energy resolution while removing the need to over-bias the detectors, is planned for May 2007. Both the recently completed and the planned experiment have significantly benefited from the developments and insights that resulted from Dr. Bleuel's work. Support for current activities in the area of Surrogate experiments comes from programatic sources, the Lawrence Fellowship fund, and the Stockpile Stewardship Academic Alliance program.

3.9 Experiments in the mass 90-104 region

In November 2003, a test experiment was carried out at Yale by L. Ahle, L. Bernstein, and J. Church, in collaboration with the Academic Alliance group at Yale. The ^{92}Zr(α,α') experiment, a Surrogate for n-induced reactions on ^{91}Zr, served as a commissoning run for the particle detector STARS and facilitated the development of data analysis routines which were needed for subsequent Surrogate experiments. A second experiment, which featured the ^{92}Zr(d,d') reaction, was completed in May 2004. The experiments carried out at Yale University suffered, respectively, from impurities in the target and an unexpected unavailability of the helium beam, which forced the experimental group to use a deuteron beam. The analysis of the data led to the conclusion that Surrogate experiments require very clean targets with carefully selected backings or (preferably) without backing.

Subsequently, a new and improved experimental setup was developed, installed, and tested at Lawrence Berkeley National Laboratory (LBNL) in Fall/Winter 2004. A set of new experiments was planned in order to establish benchmarks for the Surrogate approach and to extract unknown cross sections in the mass 90-104 region. Special emphasis was placed on the target-making process – new targets were produced specifically for the LDRD experiments. ^{102}Ru(α,α') and ^{104}Ru(α,α') experiments, which serve as Surrogates for n-induced reactions on ^{101}Ru and ^{103}Ru, respectively, were carried out in May 2005. Unfortunately, however, the analysis of the Ru data turned out to be very challenging. Various issues related to cross talk and detector efficiencies could not be resolved. Details of the work are given in an internal report [13].

4 Further accomplishments

Apart from the technical progress that was made in the context of this LDRD project (see previous section), our activities resulted in a series of achievements that benefit the Laboratory in general and the PAT directorate in particular. Below, we highlight some accomplishments that signify increased visibility of research carried out at the Laboratory and new opportunities for collaborative work, hiring, and research funding.

4.1 Return to the Laboratory

At the beginning of the project, there had been little research activity in the area of Surrogate reactions (apart from the early intense work in the 1970s). This situation has changed during the past few years, in large part due to work carried out by N Division scientists and their collaborators. The Surrogate LDRD project, the Surrogate workshop (see Section 4.3 below), the careful analyses carried out by Younes *et al.* [41, 42], and the experimental efforts focused on the actinide region and led by L. Bernstein, have generated much interest in the Surrogate approach and increased the visibility of our research activities in this area. The Surrogate method was recently featured in the "RIA Theory Bluebook" [16], and the National Research Council's report on "Scientific Opportunities with a Rare-Isotope Facility in the United States" [35], the "Report of the Nuclear Physics and Related Computational Science R&D for Advanced Fuel Cycles Workshop" [37] and Dr. R. Orbach's address at the Global Nuclear Renaissance Summit in December 2006, "The Role of the Office of Science and AFCI" [32].

New collaborations, involving both theorists and experimentalists from the LDRD team, have formed, and we have been invited by scientists from both universities and national laboratories to participate in research projects and proposals featuring the Surrogate method. There are ongoing collaborations with experimentalists from Lawrence Berkeley National Laboratory, Yale University, the University of Richmond, and with an experimental group from Rutgers University/Oak Ridge National Laboratory led by Prof. Jolie Cizewski. Researchers at Texas A&M University have recently been awared a Stewardship Science Academic Alliance grant that involves L. Ahle and J. Escher as collaborators. We have established collaborative efforts with theorists from the University of Surrey, UK, (in particular with Prof. Ian Thompson, who was identified as a strategic hire for PAT and is now working in N Division), the CEA in Bruyères-le-Châtel (France), Oak Ridge National Laboratory, and Los Alamos National Laboratory. In collaboration with theorists at ORNL, we have recently submitted a LLNL-led proposal entitled "Surrogate nuclear reaction theory for the Advanced Fuel Cycles (PI: J. Escher)" to the Department of Energy's Office of Science [23]. A complementary proposal, experimental, that involves J. Burke and L. Bernstein, has been submitted by R. Clark *et al.* from LBNL. Also, new nuclear reactions workshop, co-organized with scientists from LANL, is planned for later this year.

4.2 Training and Recruiting

Our collaborative efforts on Surrogate reactions have provided the PAT directorate with excellent recruiting opportunities. With the LDRD funding provided for the the Surrogate research project we are able to hire and partially support three new postdoctoral researchers. During the course of the project, we had a total of five postdoctoral researchers closely collaborating with us: C. Forssen is now a researcher at Chalmers University in Sweden; J. Church and J. Burke have been hired into staff positions at LLNL, V. Gueorgiev is currently completing his term as postdoc at LLNL, and D. Bleuel, originally a postdoc at LBNL, was recently hired as a postdoc at LLNL.

Overall, the postdocs benefited greatly from the the interaction with the senior personnel at the Laboratory. In particular, the expertise and advise from the Laboratory associates was extremely valuable. In addition, in order to introduce and review the relevant concepts and tools of nuclear reaction theory, we established a set of tutorials on the topic "Surrogate Nuclear Reaction Physics". The lectures, which started in October 2003 and continued throughout the duration of the research project, were presented by experts in the fields of reaction theory and reaction experiment, both from within and from outside the Laboratory. Lecture notes and other relevant materials were made available at a Laboratory web site, http://www-phys-d.llnl.gov/Research/N_Tutorials/www/.

4.3 Workshop on Surrogate reactions

Indirect approaches for studying nuclear reactions, and the Surrogate method in particular, were the focus of a workshop we organized during the first year of this LDRD project. The local organizing committee included the Surrogate LDRD team and was chaired by the principal investigator (J. Escher). The workshop, entitled "Nuclear Reactions on Unstable Nuclei and the Surrogate Reaction Technique," was held at the Asilomar Conference Grounds in Pacific Grove, California, January 12-15, 2004. The meeting attracted about 60 participants from the international nuclear structure and reaction communities. The international advisory committee included scientists from universities (MIT, Michigan State University, and Ohio University) and research laboratories (Argonne, Livermore, Los Alamos, Oak Ridge, TRIUMF in Canada, and the Commissariat à l'Energie Atomique (CEA) in France). Funding for the workshop was provided by N Division, Lawrence Livermore National Laboratory.

The three and one-half day meeting consisted of plenary talks, parallel sessions, and working group discussions. Nuclear astrophysics, stockpile stewardship science, transmutation of nuclear waste technology, and nuclear structure physics were identified as the primary areas that will benefit from new nuclear-reaction information. Workshop participants reviewed the status of current experimental, theoretical, and computational tools available for the study of nuclear reactions. The state-of-the-art in transfer-reaction theory, level-density calculations, pre-equilibrium reaction studies, etc. was discussed and opportunities at radioactive beam facilities were outlined. The ANC (Asymptotic Normalization Coefficient) method, which has been applied to peripheral capture reactions in recent years, was presented as an example of an indirect technique for determining reaction cross sections. The workshop participants also learned about a new program of indirect nuclear spectroscopy studies at Oak Ridge, which employs radioactive ion beams to carry out (d,p) reactions in inverse kinematics.

At the center of the discussions was the Surrogate-reaction technique. Early applications of the method, the more recent studies by Younes and Britt, as well as some test experiments carried out by Bernstein *et al.* were critically examined at the workshop. Working groups were formed to discuss possible applications and practical limitations of the Surrogate technique, to explore various technical issues associated with implementing the method, and to develop strategies for making progress.

The consensus at the meeting was that reactions on unstable nuclei are very important and that indirect methods will play an essential role in their study. The Surrogate approach was recognized as a potentially very useful and in some circumstances the only feasible method for obtaining unknown cross sections. The need for careful studies of the method was emphasized and the importance of establishing benchmarks was stressed. The workshop participants also contemplated the future of nuclear reaction physics. In this context, attracting young researcher to the field and strengthening collaborations between universities and research laboratories were identified as important goals. Overall, the presentations and discussions at the workshop illustrated nicely that the study of reactions on unstable nuclei is a challenging field with complex and rich physics as well as important and fascinating applications.

The viewgraphs of the individual presentations, as well as further information about the meeting, were posted on the workshop web site, www-pat.llnl.gov/Conferences/Surrogates04/ and a brief summary of the conference activities appeared in *Nuclear Physics News International* [19].

4.4 Publications and Presentations

A series of publications, reports, and presentations have resulted from the activities associated with this LDRD project. Below we include a list of articles, conference proceedings, reports, invited and contributed presentations that were prepared in the context of our Surrogate work. For the publications, we distinguish between achievements that resulted directly from the work supported with LDRD funds (indicated by the symbol ▷) and those that were partially supported by or benefited from the work carried out under LDRD. No such distinction is made for the presentations.

Refereed Articles

1. ▷ C. Forssén, F.S. Dietrich, J. Escher, R. Hoffman, and K. Kelley, "Determining neutron-capture cross sections via the surrogate reaction technique," submitted to Phys. Rev. C, 2007, UCRL-JRNL-228066.

2. L. A. Bernstein *et al.*, "Deducing the ^{237}U(n,γ) and (n,2n) Cross Sections Using a New Surrogate Ratio Method," submitted to Physical Review C.

3. J. Escher and F. S. Dietrich, "Determining (n,f) cross sections for actinide nuclei indirectly: An examination of the Surrogate Ratio Method," Phys. Rev. C 74 (2006) 054601.

4. J. Burke, L. A. Bernstein, J. Escher, et al., "Deducing the ^{237}U(n,f) Cross Section Using the Surrogate Ratio Method," Phys. Rev. C 73 054604 (2006).

5. ▷ J. Escher et al., "Surrogate Nuclear Reactions - an Indirect Method for Determining Reaction Cross Sections," Jour. Phys. G 31 (2005) S1687-S1690.

6. ▷ J. Escher et al., "Surrogate Nuclear Reactions and the Origin of the Heavy Elements," Nucl. Phys. A 758 (2005) 86c–89c.

7. ▷ J. A. Church et al., "Determining Neutron Capture Cross Sections with the Surrogate Reaction Technique: Measuring decay probabilities with STARS," Nucl. Phys. A758 (2005) 126c–129c.

8. ▷ C. Forssen et al., "Theoretical Challenges of Determining Low-energy Neutron Capture Cross Sections via the Surrogate Technique," Nucl. Phys. A758 (2005) 130c-133c.

Conference Proceedings and other Non-refereed Publications

1. ▷ F.S. Dietrich and J.E. Escher, "Compound-nuclear reaction cross sections via surrogate reactions," In *Proceedings for the IXth International Conference on Nucleus-Nucleus Collisions in Rio de Janeiro, Brazil, August 28 -September 1, 2006*, page (accepted), 2006, UCRL-PROC-225487.

2. C. Beausang et al., "New results on fission cross sections in actinide nuclei using the surrogate ratio method and on conversion coefficients in triaxial strongly deformed bands in ^{167}Lu from ICE Ball and Gammasphere," In *Proceedings for Trends in Nuclear Physics, Zakopane, Poland, September 4 - 10, 2006*, page (submitted), 2006, UCRL-PROC-227750.

3. ▷ J. Escher, F. S. Dietrich, and C. Forssén, "Surrogate nuclear reaction methods for astrophysics," *Nucl. Instr. and Meth. B*, page (accepted), 2006, UCRL-JRNL-224284.

4. ▷ C. Forssén, F.S. Dietrich, J. Escher, V. Gueorguiev, R.D. Hoffman, and K. Kelley, "Compound-nuclear reaction cross sections via Surrogate measurements," In *International Symposium on Nuclear Astrophyscs – Nuclei in the Cosmos IX , June 25–30, 2006*, volume Pos(NIC-IX), page 224, 2006, UCRL-PROC-223820.

5. J. Escher and F. S. Dietrich, "Determining compound-nuclear reaction cross sections via Surrogate reactions: Approximation schemes for (n,f) reactions," In E. Gadioli, editor, *Proceedings for the 11th International Conference on Nuclear Reaction Mechanisms, Varenna, June 12-16, 2006*, 2006, UCRL-PROC-222939.

6. J. Escher and F. S. Dietrich, "Indirect Methods for Nuclear Reaction Data," In E. Bauge, editor, *Perspectives on Nuclear Data in the Next Decade, Bruyère-le-Châtel, France, September 26–28, 2005*, 2006, UCRL-PROC-217429.

7. ▷ J. Escher and F. S. Dietrich, "Determining Cross Sections for Reactions on Unstable Nuclei: A Consideration of Indirect Approaches," In *Second Argonne/MSU/JINA/INT RIA Workshop: Reaction Mechanisms for Rare Isotope Beams (Michigan State University, East Lansing, MI, March 9–12, 2005), AIP Conference Proceedings, 791 (2005)* 93–100.

8. ▷ J. Escher et al., "The Surrogate Method - An Indirect Approach to Compound-Nucleus Reactions," In *Proceedings of the 21st Winter Workshop on Nuclear Dynamics (Breckenridge, Colorado, February 5–12, 2005)*, pp. 49–56, UCRL-PROC-211557.

9. ▷ J. Escher, "Nuclear Reactions on Unstable Nuclei and the Surrogate Reaction Technique," Meeting report on the workshop in Asilomar, Nuclear Physics News International, Vol. 14, No. 2 (2004), UCRL-JRNL-202685.

Technical Reports, Internal Memos, Etc.

1. ▷ F. S. Dietrich, "Expressions for form factors for inelastic scattering and charge exchange in plane-wave, distorted-wave, and coupled-channels reaction formalisms," Technical Report UCRL-TR-224742, Lawrence Livermore National Laboratory, Livermore, CA, 2006.

2. ▷ J. Escher, "Producing a compound nucleus via a inelastic scattering: The ^{90}Zr$(\alpha, \alpha')^{90}$Zr* case," Technical Report UCRL-TR-xxx, Lawrence Livermore National Laboratory, Livermore, CA, 2007.

3. ▷ J. A. Church et al., "Surrogate reactions towards nucleosynthesis: ^{102,104}Ru$(\alpha, \alpha'\gamma)$ as surrogate reactions for ^{101,103}Ru(n,γ)," Technical Report UCRL-TR-226860-DRAFT, Lawrence Livermore National Laboratory, Livermore, CA, 2006.

4. ▷ V. Gueorguiev, P.D. Kunz, J. Escher, and F.S. Dietrich, "^{156}Gd spin-parity distribution for the neutron-transfer reaction 156Gd(^{3}He,α)^{156}Gd at excitation energies above the neutron separation energy in ^{156}Gd," Technical Report UCRL-TR-xxx, Lawrence Livermore National Laboratory, Livermore, CA, 2007 (in preparation).

5. I.J. Thompson and J. E. Escher, "Theory of (^{3}He,α) surrogate reactions for deformed uranium nuclei," Technical Report UCRL-TR-225984, Lawrence Livermore National Laboratory, Livermore, CA, 2006.

6. ▷ F. S. Dietrich, "Simple derivation of the Hauser-Feshbach and Weisskopf-Ewing formulae, with application to Surrogate reactions," Technical Report UCRL-TR-201718, Lawrence Livermore National Laboratory, Livermore, CA, 2004.

7. J. Escher and J. Burke, "The case for initiating a R&D effort to produce targets from small material samples," LLNL Memo, UCRL-MI-219184, Lawrence Livermore National Laboratory, Livermore, CA, 2006.

8. ▷ J. Escher, "Inelastic alpha scattering on ^{102,104}Ru," LLNL N Division Memo N05-001 (May 2005).

9. J. Escher, F.S. Dietrich, I.J. Thompson, G. Arbanas, C. Bertulani, D.J. Dean, and A.K. Kerman, "Surrogate nuclear reaction theory for the Advanced Fuel Cycles," proposal submitted to the Department of Energy's Office of Science in response to the program announcement to DOE National Laboratories, LAB 07-05, *Nuclear Physics Research and Development for the Advanced Fuel Cycles*, January 2007, UCRL-PROP-227267.

Invited Conference Talks, Seminars, and Colloquia

1. J. Escher, "Nuclear reaction data from Surrogate measurements," Invited talk to be given at the *"Eighth International Topical Meeting on Nuclear Applications and Utilization of Accelerators (AccApp07)," in Pocatello, Idaho, July 30 - August 2, 2007*, 2007, UCRL-ABS-228133.

2. J. Escher, "Compound-nuclear reaction cross sections from Surrogate measurements," Invited talk to be given at the *International Conference on Nuclear Data for Science and Technology (ND2007), Nice, France, April 22-27, 2007*, 2007, UCRL-ABS-225250.

3. J. Escher, "Surrogate nuclear reaction methods for astrophysics and other applications," Invited talk at *Conference on the Application of Accelerators in Research and Industry (CAARI-2006), Fort Worth, Texas, August 20-25, 2006*, 2006, UCRL-PRES-224112.

4. J. Escher, "Surrogate reactions for advanced fuel cycles," Invited talk at *Nuclear Physics and Related Computational Science R&D for Advanced Fuel Cycles Workshop, Bethesda, MD, August 1-12, 2006*, 2006, UCRL-PRES-223747.

5. J. Escher, "Compound-nuclear reaction cross sections via Surrogate reactions," Invited talk at *11th International Conference on Nuclear Reaction Mechanisms, Varenna, June 12-16, 2006*, 2006, UCRL-PRES-222548.

6. J. Escher, "Indirect Methods for Nuclear Reaction Data," presented at the workshop *Perspectives on Nuclear Data in the Next Decade, Bruyère-le-Châtel, September 26–28, 2005*, UCRL-PRES-216143

7. J. Escher, "Nuclear Reactions with Unstable Nuclei and the Surrogate Reaction Technique," presented at the *Second Argonne/MSU/JINA/INT RIA Workshop: Reaction Mechanisms for Rare Isotope Beams, Michigan State University, East Lansing, March 9–12, 2005.*

8. J. Escher, "Nuclear Reactions with Unstable Nuclei and the Surrogate Reaction Technique," presented at the *21st Winter Workshop on Nuclear Dynamics," Breckenridge, Colorado, February 5–12, 2005.*

9. Surrogate Nuclear Reactions for Astrophysics," presented at the *RIA Theory Working Group Workshop, Tucson, Arizona, November 2-3, 2003*, UCRL-PRES-200620

10. C. Forssén, "Indirect methods in nuclear physics," Invited seminar at *T-16, Los Alamos National Laboratory, Los Alamos, NM, October 25, 2005*, 2005, UCRL-PRES-216514.

11. J. Escher, "Surrogate Nuclear Reactions: An Indirect Method for Nuclear Reaction Data," – Invited seminar, presented at Lawrence Livermore National Laboratory at the *Stockpile Stewardship Academic Alliance Meeting, February 13, 2006*, UCRL-PRES-219245.

12. J. Escher, “Cosmic Questions and Microscopic Answers: Understanding the Origins of the Heavy Elements,” – Invited colloquium, presented at Washington State University in Pullman, WA, October 25, 2005, UCRL-PRES-216460.

13. J. Escher, “Surrogate Nuclear Reactions and the Origin of the Heavy Elements,” – Invited colloquium, Lawrence Berkeley National Laboratory, September 20, 2004.

Contributed Conference Talks

1. J. Escher, “Formation of a compound nucleus following a direct reaction,” talk at the *2007 Town Meeting for NSAC Long-Range Plan, Chicago, IL, January 19-21, 2007*, 2007, UCRL-PRES-228109.

2. J. Escher, “ Compound-nuclear reaction cross sections via the Surrogate method: considering the underlying assumptions,” talk at the *2006 Annual Meeting of the DNP of the APS, October 25-28, 2006, Nashville, TN*, 2006, UCRL-ABS-222547.

3. J. Escher, “Surrogate Nuclear Reactions - An Indirect Method for Determining Reaction Cross Sections,” presented at *NUSTAR05, Guildford, UK, January 2005.*

4. J. Escher, “Nuclear Reactions with Unstable Nuclei and the Surrogate Reaction Technique,” presented at the *APS/DNP Fall 2004 Meeting, Chicago, Illinois, October 2004.*

5. J. Escher, “Surrogate nuclear reactions and the origin of the heavy elements,” presented at *The Eighth International Symposium on Nuclei in the Cosmos,” Vancouver, Canada, July 2004.*

6. J. Escher, “Surrogate Nuclear Reactions The Theory Effort at LLNL,” presented at *Nuclear Reactions on Unstable Nuclei and the Surrogate Reaction Technique,” Asilomar Conference Grounds, Pacific Grove, CA, January 11-15, 2004*, UCRL-PRES-304044

7. F.S. Dietrich, “Surrogate nuclear reactions - an indirect approach for obtaining nuclear reaction data,” Talk given at the *IXth International Conference on Nucleus-Nucleus Collisions in Rio de Janeiro, Brazil, August 28 - September 1, 2006*, 2006, UCRL-ABS-220697.

8. V. Gueorguiev , “Surrogate Nuclear Reactions,” Talk given at the *Fall 2005 Meeting of the California Section of the American Physical Society, Sacramento, California - October 21-22, 2005.*

9. C. Forssén, “Surrogate Nuclear Reactions and the Origin of the Heavy Elements,” Talk given at the *International Nuclear Physics Conference (INPC 2004),” Göteborg, Sweden, June 27 – July 2, 2004.*

Presentations to External Parties

1. C. Forssén, “Surrogate Nuclear Reactions for Astrophysics and SBSS,” Presentation to the PAT Directorate Technical Review Committee, LLNL, February 2005
2. J. Escher, “Surrogate Nuclear Reactions for Astrophysics and SBSS,” Presentation to the PAT Directorate Technical Review Committee, LLNL, December 15, 2003
3. J. Escher, “Surrogate Nuclear Reactions and the Origin of the Heavy Elements,” Presentation at the LLNL-MSU Meeting on RIA, N Division, LLNL, October 2, 2003

Poster Presentations

1. “Compound-nuclear Reaction Cross Sections via Surrogate Measurements” – Poster presentation to be given by C. Forssén at the “International Symposium on Nuclear Astrophysics - Nuclei in the Cosmos IX”, CERN, Geneva, Switzerland, June 25-30, 2006
2. “Cosmic Questions and Microscopic Answers: Understanding the Origins of the Heavy Elements,” – invited poster presented at the “2004 Laboratory Women’s Forum,” Berkeley, California, October 2004.
3. “The Surrogate Method for Reaction Cross Sections” – Poster presentation given by V. Gueorguiev at the FY2005 PAT Postdoc Symposium, December 2004. UCRL-POST-208192
4. “Determining Neutron Capture Cross Sections with the Surrogate Reaction Technique: The Angular-momentum Mismatch and Other Theoretical Challenges” – Poster presentation by C. Forssén at the “The Eighth International Symposium on Nuclei in the Cosmos,” Vancouver, Canada, July 2004. UCRL-POST-205232
5. “Determining Neutron Capture Cross Sections with the Surrogate Reaction Technique: Measuring Decay Probabilities with STARS” – Poster presentation by J. A. Church at the “The Eighth International Symposium on Nuclei in the Cosmos,” Vancouver, Canada, July 2004. UCRL-POST-205242
6. “Surrogate Nuclear Reactions and the Origin of the Heavy Elements” – Poster presentation given by C. Forssén at the 2004 PAT Postdoc Symposium, January 8, 2004.

5 Outlook and exit strategy

LDRD funding for the Surrogate research project has enabled significant progress in an area of nuclear physics that encompasses exciting and complex basic science and, in addition, has significant impact on applications in national security, energy, and astrophysics. A qualitative and quantitative understanding of nuclear reactions with unstable targets is crucial for such applications and the Surrogate method provides opportunities for determining reaction information that is otherwise very difficult or impossible to obtain.

The relevance of the Surrogate approach to several different areas of application enables us to seek funding from various possible sources. For example, L. Bernstein is leading an ongoing DNT/NA-22-funded program of Surrogate measurements in the actinide region, that also provides support for J. Burke and F. Dietrich. J. Escher receives support from ASC/PDRP for theoretical work on Surrogate reactions for actinide nuclei. Theorists from the LDRD team are also involved in a recently funded SciDAC-2 research project that includes the exploration of issues crucial to formulating reliable cross section predictions.

In addition to the (partial) support we are currently receiving for research related to Surrogate reactions, we are also seeking new funding, e.g. from the Department of Energy's Office of Science. The Surrogate method was recently identified as an important approach for application in the area of Advanced Fuel Cycles. The method was featured in a report summarizing the results of a DOE-organized workshop on *Nuclear Physics and Related Computational Science R&D for Advanced Fuel Cycles* [37] as well as in Dr. R. Orbach's discussion of the role of the Office of Science and AFCI at the Global Nuclear Renaissance Summit in December 2006 [32]. In response to a call for proposals by the Office of Science, we submitted a LLNL-led proposal entitled *Surrogate nuclear reaction theory for the Advanced Fuel Cycles* that inolves J. Escher (PI for the proposal), I.J. Thompson, and F.S. Dietrich from LLNL, as well as theorists from ORNL [23]. A complementary experimental proposal, that involves J. Burke and L. Bernstein, has been submitted by R. Clark *et al.* from LBNL.

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